

An approach for solvent selection in extractive distillation systems including safety considerations

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Table S1. Properties for the solvents considered as candidates for entrainers.

NAME	Octanol/ Water partition coef.	Flash Temperature (open cup) (K)	Enthalpy of Vaporization (kJ/mol)	Normal Boiling point (K)
1,2-Propylene Glycol	-0.43	377.81	67.42	445.49
1,3-Propylene Glycol	-0.387	381.08	69.84	453.47
2,3-Butanediol	0.031	387.37	69.66	458.25
1,2-Butanediol	0.0742	390.44	72.07	465.76
Diethylene Glycol	-1.07	404.62	77.31	486.71
2-(2-Methoxy) Ethanol	-0.634	358.22	63.7	467.7
1,4-Butanediol	0.117	393.4	74.49	473
Neopentylglycol	0.392	399.54	74.7	477.43
2,4-Pentanediol	0.535	399.51	74.31	477.35
2-(2-ethoxy)Ethanol	-0.199	364.73	64.38	473.03
1,5-Pentanediol	0.622	405.02	79.14	490.83
Hexylene glycol	0.853	408.35	76.94	488.39
Dipropylene glycol	-0.147	421.65	81.79	507.19
Dipropylene glycol Mono methyl ether	0.374	381.21	73	502.75
1,6-Hexanediol	1.13	416.05	83.79	507.22
Ethylene glycol	-0.78	383.69	62.46	429.52
Dimethyl-formamide	-0.35	-	38.78	345.13

Table S2. Optimal design obtained for the extractive distillation process using each solvent

ϵ	NT_e	FS_e	SS_e	Solvent Flow, 10^{-2} (Kmol/s)	NT_r	FS_r	P_1 (bar)	P_2 (bar)	DD_{aver} (m/yr)	TAC (\$/yr)
<i>Dimethylformamide</i>										
<i>Min DD_{aver}</i>	48	38	6	0.8212	21	11	1.00	1.00	0.18525	1036785
<i>1.908</i>	47	37	6	0.8212	19	10	1.00	1.00	0.18523	1031803
<i>1.964</i>	44	36	8	0.8212	19	10	1.00	1.00	0.18652	1028731
<i>2.020</i>	42	35	7	0.7812	18	10	1.02	1.05	0.18662	1025334
<i>2.076</i>	42	33	8	0.7489	18	10	1.09	1.05	0.18840	1022439
<i>2.132</i>	32	24	8	0.7540	18	8	1.31	1.32	0.19535	1017354
<i>min TAC</i>	44	36	6	0.8212	19	11	1.00	2.96	0.21885	1013846
<i>Diethylene glycol</i>										
<i>Min DD_{aver}</i>	48	40	22	3.501	20	15	1.00	1.00	0.26259	571142
<i>2.979</i>	42	38	5	4.526	19	16	3.49	1.13	0.29774	507459
<i>3.333</i>	48	41	25	3.501	14	9	6.72	1.53	0.33245	495370
<i>3.686</i>	45	39	3	3.501	20	15	5.71	3.75	0.36845	490365
<i>4.040</i>	41	38	20	3.463	18	12	6.42	5.73	0.40363	486241
<i>4.393</i>	43	39	17	3.245	21	14	8.16	7.27	0.43540	486678
<i>min TAC</i>	40	35	9	4.538	22	13	8.50	10.32	0.47465	484629
<i>Dipropylene glycol</i>										
<i>Min DD_{aver}</i>	50	41	4	4.328	12	7	1.00	1.00	0.23031	596486
<i>2.589</i>	47	44	2	4.526	12	8	2.13	1.75	0.25851	512807
<i>2.875</i>	42	40	13	4.526	11	7	6.00	1.75	0.28670	500330
<i>3.161</i>	47	41	3	4.526	11	7	10.00	2.16	0.31608	492472
<i>3.447</i>	50	44	5	6.835	9	5	12.55	3.00	0.34459	485783
<i>3.733</i>	47	42	3	4.526	10	6	12.85	5.27	0.37294	484286
<i>min TAC</i>	37	33	5	4.526	19	12	9.02	9.62	0.40004	483130
<i>Ethylene glycol</i>										
<i>Min DD_{aver}</i>	23	21	7	0.7188	9	5	1.00	1.01	0.20521	825035
<i>0.2126</i>	22	19	5	0.7188	9	5	1.55	1.01	0.21237	809654
<i>0.2176</i>	22	18	5	0.7200	9	5	1.86	1.01	0.21584	805694
<i>0.2238</i>	22	18	6	0.7200	9	5	2.56	1.01	0.22328	800838
<i>0.2300</i>	22	18	7	0.7200	9	5	3.31	1.01	0.22997	798218
<i>0.2362</i>	22	18	7	0.7200	9	5	4.01	1.01	0.23617	797518
<i>min TAC</i>	22	17	9	1.137	10	5	4.84	1.01	0.24243	791866

Note on the subindexes: e refers to the extractive column; r refers to the solvent recovery column